MLS000736649

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 207 °C

Global applicability domain: Inside

Local applicability domain index: 6.17e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

Image not found
1,10-Phenanthroline, 2,9-dimethyl-
Measured: 160
Predicted: 121

Image not found
Ellipticine
Measured: 313
Predicted: 195

Image not found
1,10-Phenanthroline
Measured: 117
Predicted: 127

Image not found
4,7-Phenanthroline
Measured: 177
Predicted: 128

Image not found
1,10-Phenanthroline, 3,4,7,8-tetramethyl-
Measured: 279
Predicted: 117